Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 6/13/2017 5:23:59 PM
To: Washington, John [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=fdc3e8ce9f1d45c4894881ff420ca104-Washington, John]
CC: Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: RE: your convention on mass defect

I agree.

Mark

From: Washington, John
Sent: Tuesday, June 13, 2017 12:06 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Subject: RE: your convention on mass defect

Thanks, I could see that you still get the separation. I like your way better. That way, if you stay with IUPAC C=12.0000, zero divides the positive from the negative defects . . . I like having the zero benchmark.

From: Strynar, Mark
Sent: Tuesday, June 13, 2017 12:02 PM
To: Washington, John <Washington.John@epa.gov>
Cc: Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Subject: RE: your convention on mass defect

You can do it either way. We generally round to the nearest whole number and subtract it from the accurate mass. Thus all the PFAS (or most) are negative values. The other way you simply have a bunch of values that start with 0.9xxx. It does not really matter it is just a way to see things that stand out from the bulk. Seth's paper SI (attached) tells how we did it for his Decatur water work to make Kendrick Mass Defect plots.

Mark

From: Washington, John
Sent: Tuesday, June 13, 2017 11:52 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Cc: Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Subject: your convention on mass defect

Hey Mark and Andy,

When you guys calculate mass defect, do you round to the nearest whole number (so XXX.9XXX would have a mass defect of -0.1YYY) or do you round down (so XXX.9XXX would have a mass defect of 0.9XXX)?

In one of Mabury's Supporting Info, they say always round down, but I thought I would check on what you guys do.

Thanks,
John

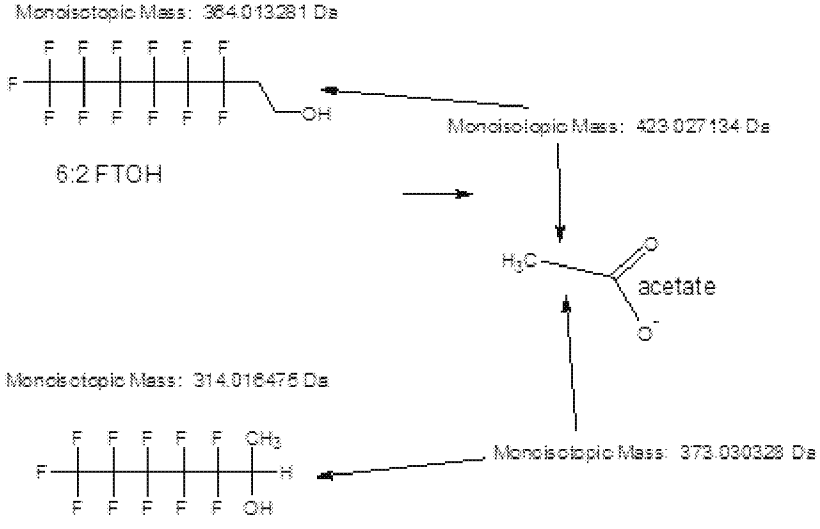
From: Strynar, Mark
Sent: Monday, June 12, 2017 8:58 AM
To: Libelo, Laurence <Libelo.Laurence@epa.gov>; Washington, John <Washington.John@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Cc: Lynch, David <Lynch.David@epa.gov>; Tobias, David <Tobias.David@epa.gov>; Antwi, Frank <antwi.frank@epa.gov>; Lee, Mari <Lee.Mari@epa.gov>; Card, Marcy <Card.Marcy@epa.gov>; Orentas, Nerija <Orentas.Nerija@epa.gov>; Wong, Eva <Wong.Eva@epa.gov>; Wong, Edmund <Wong.Edmund@epa.gov>
Subject: RE: Request for help from ORD

See my comments attached.

The 6:2 FTOH and the 5:2 sec FTOH will exist as acetate adducts of the alcohol in the QTOF in neg ESI mode.

Also their assessment of what was in the sample was 1) based on looking for what they already know to be there 2) suffers from very high LOQs 3) did not do a very good job of identifying other analytes beyond what was already known.

Polyfluorinated compounds have a unique mass defect due to multiple F and O presence in structures. With accurate masses between XXX.9XXX and XXX.05XXX it is very likely polyfluorinated and important.
Mark



From: Libelo, Laurence
Sent: Monday, June 12, 2017 7:25 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>; Washington, John <Washington.John@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Cc: Lynch, David <Lynch.David@epa.gov>; Tobias, David <Tobias.David@epa.gov>; Antwi, Frank <antwi.frank@epa.gov>; Lee, Mari <Lee.Mari@epa.gov>; Card, Marcy <Card.Marcy@epa.gov>; Orentas, Nerija <Orentas.Nerija@epa.gov>; Wong, Eva <Wong.Eva@epa.gov>; Wong, Edmund <Wong.Edmund@epa.gov>
Subject: Request for help from ORD
Importance: High

Guys,

As you know we have required a lot of biodegradation and abiotic degradation studies of fluoro polymers submitted through the new chemicals program.

One company is trying develop methods for identifying impurities and residuals in telomer based polymers and to look for possible degradation products. They have had EAG (formerly Wildlife international) use the QTOF to see what it can do. I think this is Ning Wang's work since he is now at EAG having left DuPont/Chemours.

Can you please take a look at this report from EAG on their trial of using the QTOF to look at polymers used in degradation studies. What do you think? Are their LOQ reasonable? It looks like their standard curves could be go lower. And their standard peaks are well above the noise.

Would you agree with their unknown analysis?

Other thoughts?

Thanks.

Laurence